

Message

From: McCord, James [mccord.james@epa.gov]
Sent: 10/15/2020 8:23:19 PM
To: Strynar, Mark [Strynar.Mark@epa.gov]; Leung, Lam-Wing H [LAM.H.LEUNG-1@chemours.com]
Subject: RE: Mead's paper

I've looked it over but haven't analyzed the data in depth. I did notice they implied that they were reporting BP2 isomers for the first time, but our paper pretty clearly showed a doublet with identical MS/MS fragments (it's SI figure 73-75). I have no reason to believe the constitutional isomers they suggest are separable by chromatography, but I don't know whether the stereoisomers are more separable or if it is a different structural isomer (like linear/branch on the central -OC3F6O-).

Their NVHOS analysis literally repeated the work I did. As you may recall our initial structure differed from yours based on the presence of diagnostic fragments. There are two fragments that should be incompatible but we saw them both in the standard that you shared with us. If that standard is pure then I think the isomers are indistinguishable via MS/MS alone. On the Orbitrap especially I have found the gas phase molecular rearrangements of the ether fragments to be particularly annoying, and not just from these compounds either.

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James McCord

From: Strynar, Mark
Sent: Thursday, October 15, 2020 3:44 PM
To: Leung, Lam-Wing H <LAM.H.LEUNG-1@chemours.com>; McCord, James <mccord.james@epa.gov>
Subject: RE: Mead's paper

The paper is on my list of things to read then to chat with him. I have done neither yet.

Mark

From: Leung, Lam-Wing H <LAM.H.LEUNG-1@chemours.com>
Sent: Thursday, October 15, 2020 2:12 PM
To: Strynar, Mark <Strynar.Mark@epa.gov>; McCord, James <mccord.james@epa.gov>
Subject: Mead's paper

Hi Mark & James,

Have you folks had a chance to look at this paper from Mead? I'm quite certain the "BP2" isomers he's referring to is indeed stereoisomers and not constitutional isomers as claimed in the paper. As to his observed NVHOS isomers, I'm not certain that is in agreement with our MS but I recall you looked into it. Your thoughts?

Best,
Lam

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